Special Feature 2001

Detontion Products Equation of State

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I have developed a new hybrid Monte Carlo method that allows the direct simulation of detonation products for "real" explosives such as HMX, TATB, PBX 9501, and PBX 9502. Chemical equilibrium composition, solid carbon, and phase separation are included. Now, the entire problem of interest can be simulated instead of just isolated portions as benchmarks for approximate perturbation methods.

The method is called a hybrid because the solid carbon is incorporated as an analytic model, while the fluid components are explicitly included in the Monte Carlo simulation. Chemical reactions are included as a correlated interchange of atoms between molecules. For the case of a solid carbon product, a virtual particle is created with an acceptance probability including the Gibbs free energy of the carbon. Preliminary results for HMX products with carbon in the graphite phase are shown in the figures. The statistical variation of composition in a simulation is shown in Figure 1. The dependence of composition on cross potentials is shown in Figure 2. Forthcoming high temperature diamond cell data from C-6 will be used to determine proper cross potentials.

Parallel work continues on chemical equilibrium perturbation theory methods for detonation products. My new treatment of surface chemistry on diamond clusters was published: M. Sam Shaw, "A Theoretical Equation of State for Detonation Products with Chemical Equilibrium Composition of the Surface of Small Carbon Clusters," *Shock Compression of Condensed Matter* - 1999, p. 235 (2000). This model is currently being incorporated in the hybrid MC.

I have revised and improved my data analysis methods for inverting precision DX-1 velocimetry data to obtain very accurate EOS isentropes. This includes a regional fit that incorporates multiple data sets and gives derivative information such as Gruneisen gamma. Joint papers with DX-1 are: R. S. Hixson. M. S. Shaw, J. N. Fritz, J. E. Vorthman, and W. W. Anderson, "Release Isentropes of Overdriven PBX-9501," *J. Appl. Phys*. (accepted for publication), and J. E. Vorthman, R. S. Hixson, W. W. Anderson, J. N. Fritz, and M. S. Shaw, "Release Isentropes in Overdriven PBX 9502," *Shock Compression of Condensed Matter* - 1999, p. 223 (2000). These results provide very important constraints on the EOS models described above. The SESAME tabular EOS form is being used to make both experimental and theoretical results available to hydrodynamics calculations.

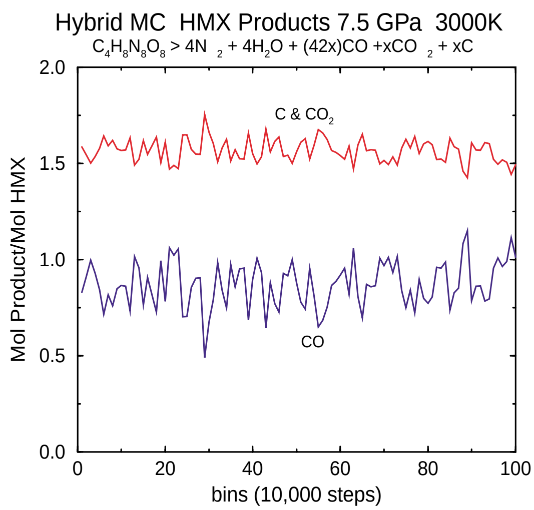

Figure 1: Statistical variation of composition in a simulation.

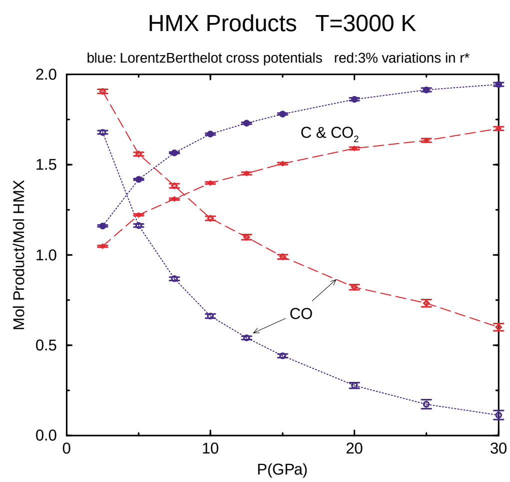

Figure 2: Dependence of composition on cross potentials.

This paper is a portion of LA-UR-01-1847, May 2001 .